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Significant contributions in algorithms and codes for automatic grid generation were made in the following specific areas: automatic generation of multidimensional Fortran code via Symbolic Manipulation (Artificial Intelligence), requiring user input of only the governing partial differential equations or the governing variational principles; rigorous techniques for verification of codes, algorithms, and discretization methods; a new and effective formulatin for variational methods; analysis of mathematical properties (ellipticity, convexity) of PDE and variational methods including volume, orthogonality, smoothness and other controls; identification and explanations of previously unreported anamolies in common grid generation algorithms, including non-uniqueness due to solution bifurcation and grid folding; identification and explanation of previously unreported ambiguities in common discrete evaluations of transformation Jacobians; use of a reference grid to control target grid properties; development of a solution adaptive method for surface grid generation; development of a hybrid method of solution adaptive grid generation which properly isolates the multigrid methods to elliptic grid generation; development of an algorithm for econmically generating sub-grid grid generation discretization required for multigrid solution techniques; correct interpretation of the "smoothness" property of elliptic grid generation.

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FINAL SCIENTIFIC REPORT FOR CONTRACT F49620-84-C-0079

"ADAPTIVE GRID GENERATION USING ELLIPTIC GENERATING EQUATIONS WITH PRECISE COORDINATE CONTROLS"

ECODYNAMICS RESEARCH ASSOCIATES, INC.
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8 JULY 1992

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ABSTRACT

Significant contributions in algorithms and codes for automatic grid generation were made in the following specific areas: automatic generation of multidimensional Fortran code via Symbolic Manipulation (Artificial Intelligence), requiring user input of only the governing partial differential equations or the governing variational principles; rigorous techniques for verification of codes, algorithms, and discretization methods; a new and effective formulation for variational methods; analysis of mathematical properties (ellipticity, convexity) of PDE and variational methods including volume, orthogonality, smoothness, and other controls; identification and explanation of previously unreported anamolies in common grid generation algorithms, including non-uniqueness due to solution bifurcation and grid folding; identification and explanation of previously unreported ambiguities in common discrete evaluations of transformation Jacobians; use of a reference grid to control target grid properties; development of a solution adaptive method for surface grid generation; development of a hybrid method of solution adaptive grid generation which properly isolates the contribution of the adaptivity functional; application of multigrid methods to elliptic grid generation; development of an algorithm for economically generating sub-grid grid generation discretizations required for multigrid solution techniques; correct interpretation of the "smoothness" property of elliptic grid generation.

B. STATEMENT OF WORK

"The contractor will develop, verify and exercise Symbolic Manipulation codes and Fortran codes for solution-adaptive grid generation for two dimensional and three dimensinoal internal and external flows. The methods and results produced under the proposed contract will be documented in open literature and engineering meetings, and sample codes will be made available to interested users within Government agencies and their contractors."

C. STATUS OF THE RESEARCH, and D. TECHNICAL JOURNAL PUBLICATIONS.

The algorithms, mathematical analyses, and engineering applications outlined herein were developed under the subject contract and its predecessor (F49620-82-C-0064, same title). The original intention of AFOSR was to simply extend the earlier contract; this failed only because of a backlog at the AFOSR contracts office at the time. Consequently, the division of results between the two contracts is somewhat vague scientifically. Reference should also be made to the earlier work reported in the Ecodynamics Final Scientific Report on the previous contract dated 10 May 1986.

In addition to journal publications, two books eventually resulted from the work begun under sponsorship of the subject contract (as well as collateral funding).

The first book is "Mathematical Aspects of Numerical Grid Generation", No. 8 in the SIAM Series "Frontiers in Applied Mathematics", edited by Dr. Jose' E. Castillo. Dr. Castillo was partially supported by the subject contract as an Ecodynamics employee while he was successfully pursuing his Ph.D. in Mathematics. The Principal Investigator, Dr. P. J. Roache, and Dr. S. Steinberg were his co-advisors. Five of the ten chapters of this book were written by Ecodynamics personnel.

The second book is "Fundamentals of Grid Generation" by P. M. Knupp and S. Steinberg. Still in manuscript form, it is expected to be published in 1993, probably by SIAM.

The most economical and meaningful method of summarizing the results of the contract work is to simply duplicate herein the title page, including the technical abstract, for the publications supported by the subject contract. These follow.

Directly Supported Publications.

AIAA'85

AIAA-85-1527

A New Approach to Grid Generation Using a Variational Formulation

P.J. Roache and S. Steinberg

AIAA 7th Computational Fluid Dynamics Conference

July 15-17, 1985/Cincinnati, Ohio

85-1527

A NEW APPROACH TO GRID GENERATION USING A VARIATIONAL FORMULATION [1]

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Abstract

This paper reports on three aspects of grid generation. First, two behavioral errors in elliptic gird generation that are of critical importance in choosing a grid generation method are discussed. Next, a geometric continuation method for avoiding difficulties sometimes encountered in difficult geometries is described. Finally, a significant extension of the existing variational grid generation methods is described.

Background

We present here a brief background of elliptic grid generation relevant to the present work. Winslow (Ref. 1) used homogeneous Laplace equations written in the physical plane for grid generation. These equations are transformed to the logical plane where they are solved numerically. The concept behind this approach was based on the utilization of the well-known maximum principle for linear elliptic equations. The maximum principle for the Laplace equation guaranteed that the method would always produce a minimally acceptable grid, i.e. one for which the grid lines would not leave the region. Solving the equations in the transformed, or logical plane, is advantageous due to a simplification of the boundary conditions. However, this occurs at the expense of a nonlinear coupling of the governing equation. Winslow used a discretization on a triangular grid.

Hirt, Amsden, and Cook (Ref. 2) used Laplace equations written in the logical plane itself. Here, the maximum principle does not help, so the continuum formulation has no guarantee of a minimally acceptable grid. However, the method is linear and the Laplace equations are uncoupled. The method was able to produce usable solutions in some cases.

Thompson, Thames, and Mastin (TTM method, Ref. 3) extended the Winslow method by introduction of nonhomogeneous terms in the physical plane, followed by transformation to the logical plane. This resulted in a much more complicated nonlinear equations, but the right-hand side or nonhomogeneous terms allows control of the grid at interior points. The control achieved by the nonhomogeneous terms is very indirect; several papers have been published on the forms of the nonhomogeneous terms, which are strong and typically greatly slow the iterative convergence rate. See, for example, Sorenson and Steger (Ref. 4), Middlecoff and Thomas (Ref. 5), Ghia et al (Ref. 6) and Brackbill and Saltzman (Ref. 7). We note that the introduction of the nonhomogeneous terms means that the maximum principle no longer applies, especially if the sign of the nonhomogeneous term changes within the domain.

Brackbill and Saltzman (Ref. 7) approached the grid generation problem using a variational formulation of the three properties of smoothness, cell volume, and orthogonality, written in the physical plane and then transformed to the logical plane. The variational principal for smoothness alone, properly defined, leads to the Winslow equations (or the homogeneous Thompson-Thames-Mastin equations). Weighting factors are introduced to allow the user to balance the importance of these three properties. The particular weighting of orthogonality used in Ref. 7 is somewhat arbitrary, but simplifies the mathematics of the transformation.

Behavioral Errors in Grid Generation

We have encountered some elementary aspects of elliptic grid generation which bear on the selection of an existing method and on the direction of the research for our new methods.

These errors fall under the category of "behavioral errors" (Ref. 8), i.e. qualitative differences between the discretized equations and the continuum equations. This genre of classification is well-known in CFD and includes (mass) conservation errors, vorticity and enstrophy conservation errors, phase errors, artificial viscosity errors, positivity errors (e.g., local appearance of negative values for positive definite qualities such as temperature and density). Other branches of computational physics, e.g., electromagnetics, experience analogous errors.

The first behavioral error is in the evaluation of cell volume and grid folding using a discretized Jacobian. Let the mapping from the logical plane to the physical plane be given by $x = x(\xi,\eta)$, $y = y(\xi,\eta)$. In 2D, the sign of the Jacobian,

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1 Work supported partially by the U.S. Air Force Office of Scientific Research and the U.S. Army Research Office.

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AIAA'84

AIAA-84-1655

Interactive Electric Field Calculations for Lasers

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AIAA 17th Fluid Dynamics, Plasma Dynamics, and Lasers Conference

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INTERACTIVE ELECTRIC FIELD CALCULATIONS FOR LASERS[1]

by

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W. M. Moeny[3]

and

Stanly Steinberg[4]

Abstract

The goal of the computational effort described herein is to develop computer codes for rapidly and accurately modeling the electric fields in the cavity of lasers and switches. The designer is able to interactively perturb the laser operating parameters and/or electrode geometry, and quickly obtain new solutions. The codes use automatic generation of solution-adaptive boundary-fitted coordinate systems, and solve two- and three-dimensional problems in both steady-state and time-dependent modes.

Introduction and Overview

The design of electrodes for lasers and switches is well-defined only for unrealistically idealized conditions. The frequently used Rogowski electrode shapes are "optimal" only in the sense of producing an enhancement factor of unity, i.e., the electric field strength is no where greater than the nominal value. More importantly, the solution is based on vacuum conditions and is not a complete specification, i.e., the Rogowski shape is not closed, and must be completed by some (usually arbitrary) closure such as blending with a radius, etc. The same is true of the Chang electrodes.

The computer codes described herein address the realistic electrode design problem, including non-vacuum operation and complete electrode specification with "packaging" constraints of overall size. Using efficient finite difference methods in boundary-fitted coordinates, the ELF (ELectric Field) code makes it practical to design the electrode geometry and laser operating parameters during user-interactive sessions on a VAX computer. A single code is used for all 2-D calculations, both steady state and time dependent. Options are available for either the planar, axisymmetric, or radial electrode geometries. Boundary conditions and boundary shapes may be time dependent; in particular, an external circuit equation is provided so that electrode potential may be calculated as part of the solution, dependent on the integrated current through the cavity, rather than being specified a priori. The geometry and conductivity calculations are modularized so that they may be readily modified by the user.

Automatic grid generation is performed interactively using elliptic generating equation techniques. As an option, a solution adaptive grid generation technique is used to adapt the grid to the solution (either in the steady state solution, or within an intra-time-step iteration for a time-dependent problem) so as to increase the resolution of the maximum electric field strength (always an important design parameter) and the accuracy.

The code accounts for externally controlled or self-sustained glow discharges or other plasmas, such as arcs, by modifying the nonlinear conductivity. Various empirical formulations for (steady) electrical conductivity have been evaluated using the code. While somewhat useful, this approach has now been abandoned. A more fundamental approach has been adopted, that of solving for the conductivity by time integration of the ordinary differential equations for electron number density equation at each mesh point in the 2D or 3D grid, coupled nonlinearly to the local E-field. The electron drift velocities, etc., are obtained by table look-up of Boltzmann code solutions performed beforehand (i.e., noninteractively) for the particular gas mixture used. Code applications have included pulsed electric CO_2 lasers and a xenon flashlamp. For xenon flashlamp calculations and for streamer calculations, the temperature is also solved at each node point by time integration of an energy equation. Calculations have shown some insight into streamer formation in plasma discharges, the unsteady development of a self-sustained glow discharge, and lensing effects due to nonuniformities in external ionization sources.

For many cases studied, we find the electric field solutions to differ significantly from vacuum calculations, indicating that the commonly used Rogowski solutions and Chang solutions for the electrode shapes are far from optimal for important classes of problems. The true optimal geometry is, in fact, a strong function of the laser physics and of the operating conditions whenever significant physics are involved in the conductivity. Also, different lasers may have different optimality criteria; e.g., an electron-beam laser may be designed to give nearly uniform energy deposition in the cavity, whereas a self-sustained CO_2 laser may be designed to minimize the local extrema of the electric field strength, subject to external packaging geometry constraints, so as to minimize arcing and maximize the operating voltage.

Three-dimensional calculations are done in a separate code and are used only to design the roll-off of the electrodes in the third dimension so as not to produce a locally high electric field due to 3-D effects.

[1]Work supported partially by the U.S. Air Force Weapons Laboratory, the U.S. Air Force Office of Scientific Research, and the U.S. Army Research Office.

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Symbolic Manipulation and Computational Fluid Dynamics

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This paper is divided into three sections. The first section is a brief present presentation of the powerful capabilities of the symbolic manipulation code MACSYMA developed at MIT. The second section presents results recently achieved by the authors using symbolic manipulation on the problem of three-dimensional body-fitted coordinates. The third part of the paper surveys previous uses of symbolic manipulation in computational fluid dynamics and related areas, and potential future uses of the code.

Introduction

THE purpose of this paper is to provide a brief introduction to the uses of symbolic manipulation within the practice of disciplines such as computational fluid dynamics (CFD). The first section is a brief presentation of the powerful capabilities of the symbolic manipulation code MACSYMA. The next section presents results recently achieved by the present authors using symbolic manipulation on the problem of three-dimensional boundary-fitted coordinates. The last section consists of a short survey of previous uses of symbolic manipulation in CFD and related areas, and of what we consider to be promising areas for future use.

Symbolic manipulation performed by computer is an area that has just recently begun to be more widely appreciated and has tremendous potential. Symbolic manipulations are not floating point calculations, but symbolic operations (e.g., the chain rule differentiation) performed by computer logic. One of the earliest symbolic manipulation languages was FORMAC, which had the capability of doing simple differentiation symbolically. ALTRAN is a more powerful and later version of the symbolic manipulation language another version, "Micromath," is available on the better microcomputers. Perhaps the most powerful of the symbolic manipulation codes is MACSYMA, which has been developed over many years at the Massachusetts Institute of Technology.

MACSYMA Capabilities

The symbolic manipulation code MACSYMA has been developed through an extensive team effort. Many practitioners of computational fluid dynamics have some acquaintance, at least second-hand, with this code, but our impression is that few have an appreciation for its powerful capabilities or those of the general field of symbolic manipulation. These capabilities include variable-precision arithmetic and algebraic substitutions and simplifications, symbolic (rather than numeric) equation solving for scalars and matrices, truncated Taylor series expansions, power series, differentiation including the chain rule for single- and multivariate functions, very powerful definite and indefinite integration, taking limits of expressions, ordinary differential equation solving (closed-form solutions), and many other mathematical operations previously thought to be in the realm of human beings rather than computers. For an introduction to the subject of symbolic manipulation, see Refs. 1-3. Recently, a version of MACSYMA, called VAXIMA, has become available for the VAX family of minicomputers. Significantly, MACSYMA also has the capability of actually generating a Fortran code from symbolic mathematics in the usual scientific notation. MACSYMA is also a programming language and can concatenate alphanumeric variables.

The second author has developed a code called GEEWHIZ that demonstrates many of the impressive capabilities of MACSYMA. A sampling is included as an appendix in Ref. 21.

Three-Dimensional Boundary-Fitted Coordinates via Symbolic Manipulation

Background

Coding errors plague all computational work. The chance for coding error increases as the complexities of the problems increase. Computational fluid dynamics codes used in aerodynamics and ballistics calculations are commonly 5,000 or more lines of Fortran code in length. Codes used in nuclear reactor safety work have as many as 65,000 lines of Fortran. Although containing much complex physics, these codes are actually elementary in that they are written in very simple coordinate systems such as Cartesian, cylindrical, etc.

Recently, there has been a surge of activity in the application of coordinate transformation techniques. The proceedings of three recent conferences, two dedicated entirely to this problem[4,5] and one emphasizing it,[6] show a tremendous amount of work being done in this area. We have been impressed with the difficulty of code verification for transformed grid problems and with the complexity of three-dimensional equations written in general nonorthogonal grids. The most popular and most generally applicable coordinate transformation methods are boundary-fitted coordinate systems, which are generally nonconformal and therefore do not maintain the form of the original equations written in Cartesian or other elementary coordinates.

Overview

We have recently developed and validated symbolic manipulation codes for working a problem of considerable complexity—that of solving general second-order elliptic partial differential equations in a general (nonorthogonal) three-dimensional boundary-fitted coordinate system. We follow the approach of Thompson and his colleagues[7,8] and generate the coordinate system itself by solving elliptic partial differential equations in the transformed plane. We address

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JOURNAL OF COMPUTATIONAL PHYSICS 57, 251–284 (1985)

Symbolic Manipulation and Computational Fluid Dynamics*

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The problem of numerically integrating general elliptic differential equations in irregular two and three dimensional regions is discussed. The method used numerically computes a transformation of the given region into a rectangular region. The numerical coordinate transformation is determined by requiring that the components of the transformation satisfy inhomogeneous Laplace or more general equations. The transformation is then used to transform the differential equation and the boundary conditions to the rectangular region. The boundary value problem in the rectangular region is integrated using one of the standard methods for general elliptic equations. The use of the existing software reduces the problem to analytically transforming the given differential equation and the Laplacian to general coordinate frame and then writing subroutines that will tabulate the coefficients of these differential equations using the tabulated coordinate transformation. This method has been successfully used in two dimensions so we are concerned with the three dimensional extension of the existing codes where the major problem encountered is the volume of algebra and coding required to complete the method. To overcome these difficulties, a symbol manipulation program in VAXIMA is written that has as input the formula for the given differential equation in some natural coordinates and has as output the required FORTRAN subroutines. Because of the complexity of the resulting code, code validation was performed by systematic truncation error testing. The paper concludes with a discussion of the problems encountered in using a symbol manipulator to write large FORTRAN codes.

Contents.

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THE ELF CODES: ELECTRODE DESIGN FOR LASERS AND SWITCHES*

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The ELF (Electric Field) codes have been developed as a design tool for modeling the electric potential and field strength in the cavity of a laser or switch. In an interactive computer environment, the designer is able to perturb the device operating parameters (applied voltage, external circuit elements, gas mixture, external ionization source parameters, etc.) and/or the electrode shapes, and quickly obtain new solutions. The codes solve two- and three-dimensional problems in both steady-state and time-dependent modes. The five-year development of the codes has involved an interdisciplinary team approach of laser physicists, mathematicians, and computational engineers. The computational techniques developed and embodied in the codes involve the following areas: semidirect/marching methods for nonlinear elliptic equations, fully implicit methods for strongly coupled nonlinear time evolution equations, solution-adaptive boundary-fitted grid generation, gas conductivity modeling, parametric surface representations, super-microcomputer operations, artificial intelligence (computer symbolic manipulation), code validation procedures, software engineering for interactive codes, and numerical machining considerations. Future work may involve multi-

* Work supported partially by the U.S. Air Force Weapons Laboratory, the U.S. Air Force Office of Scientific Research, and the U.S. Army Research Office.

This paper is in final form and no version of it will be submitted for publication elsewhere.

Application of a Single-Equation MG-FAS Solver to Elliptic Grid Generation Equations (Subgrid and Supergrid Coefficient Generation)

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ABSTRACT

A single-equation MG-FAS solver is applied to elliptic grid generation equations obtained from variational principles and to problems of fluid dynamics and electromagnetics on these grids. The problem of automatic generation of subgrid coefficients, given the user defined discretized problem on a defining grid, is addressed in a novel and clear way which has some advantages. The same idea is applied to supergrid generation of the elliptic grid generation equations, which can result in substantial arithmetic savings for solution adaptive grid generation in 3D.

1. INTRODUCTION

The motivation for the present work on multigrid methods is the solution of problems in computational fluid dynamics and electromagnetics, and grid generation for these problems [1–4], in 2D and 3D. Several aspects of these problems bear on the formulation and the difficulties addressed in the present work.

The well-known high-grid-Reynolds-number phenomenon in the CFD problems [5, 6], and the corresponding phenomenon arising from rapidly varying (or even discontinuous) diffusion (conductivity) coefficients in plasma electromagnetics, can give rise to nonphysical oscillatory discretized solutions, which is aggravated by coarse grid discretization within the multigrid solution. The grid generation equations can be very complex, being based on an extension [2, 3] of the Brackbill-Saltzmann [7] variational approach. We use computer symbolic manipulation to form the variational equations, and to write FORTRAN subroutines for the stencils [8, 9]. Even in 2D, when a strong coordinate angle control (nonorthogonal) is used (e.g. to adapt to solution streamline angles) the arithmetic is very expensive, compared to that of the

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"A Tool Kit of Symbolic Manipulation Programs for Variational Grid Generation", S. Steinberg and P. J. Roache, AIAA Paper No. 86-0241, AIAA Aero-space Sciences Meeting, 6-9 January 1986, Reno, NV.

Abstract not available.

COMMUNICATIONS IN APPLIED NUMERICAL METHODS, Vol. 4, 471–481 (1988)

ON THE FOLDING OF NUMERICALLY GENERATED GRIDS: USE OF A REFERENCE GRID

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SUMMARY

When variational grid generation techniques are used to produce grids suitable for solving numerical partial differential equations in irregular geometries, a reference grid can be used to determine the properties of the desired grid. Grid folding is a major problem in all methods of numerical grid generation; this paper studies the use of a reference grid, in variational smoothing methods, to prevent such foldings. The effects of various types of reference grid are compared and natural reference grids are shown to prevent foldings in the examples studied. The analysis is performed for a model problem with only one free point, and is then applied for finer grids. In addition, a short description of a discrete variational method is given. The reference grid concept applies to this discrete formulation.

INTRODUCTION

Grid folding is one of the main concerns in numerical grid generation. In this paper we analyse a variational grid generation method that uses a reference grid as a tool in preventing such folding. A reference grid is a region somewhat like the physical region where the grid is to be placed but which can be much simpler (see Figure 1). The idea is to define, on the reference grid, the properties of the grid which we want to transfer to the given physical object.[1] (It is worth noting that the reference grid is not limited to the determination of the grid properties in the interior of the geometric object, but also can be used to determine the grid properties on the boundary.[1])

In this paper we are considering two of the integrals from the variational methods introduced by Steinberg and Roache,[1] which are similar to the methods of Brackbill and Saltzman;[2] the two functionals presented provide (1) the measure of spacing between the grid lines (smoothness) and (2) the measure of the area of the grid cells. The minimization problem is usually solved by calculating the Euler–Lagrange (E–L) equations for the variational problem; the computer creates a grid by solving a centred finite difference approximation for the Euler–Lagrange equations.

Our study is motivated by the fact that the Winslow[3] grid generator (homogeneous TTM[4]) produces folded grids in certain electrode configurations.[5,6] In these configurations, the regions studied were roughly like the region between two concentric ellipses; the grid was 100×15. It was demonstrated that the folding was not due to nonlinear effects or coding error. The folding is intrinsic to the Winslow[3] (or homogeneous TTM[4]) method when applied to certain geometries, for finite grid sizes. Although the theorem of Mastin proves that the grids will not fold in two dimensions[8] or three dimensions[9] in the continuum limit, the results of Roache and Steinberg[5] conclusively and succinctly demonstrated that the theorem does not apply for finite mesh increments. The difficulty manifested itself even in the simplest possible grids and the results for the simple grids proved relevant to more complex and finer resolution cases (see References 5, 9 and 10). When only 3×3 grids are considered, as the case for the present analyses, the region degenerates to the area between two triangles, as in Figure 3.

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ON THE FOLDING OF NUMERICALLY GENERATED GRIDS

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Technical Report #2

July 7, 1987

ON THE FOLDING OF NUMERICALLY GENERATED GRIDS[1]

by

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Abstract

In numerical grid generation, having a grid fold is a major problem. This paper studies techniques for preventing such grid foldings. The analysis is done for a model problem with the simplest possible numerical grid, one where there is only one point to be determined.

1 Introduction

Our main interest is to study the grid generation techniques introduced by Steinberg and Roache in [1, 2]. These techniques are variational and are closely related to the techniques introduced by Brackbill and Saltzman in [3]. We will also compare the variational methods to a simple version of a method introduced by Thompson, et.al [4]. There are three basic properties to be controlled in a grid: smoothness, cell area or volume, and orthogonality. These properties are represented by integrals which are to be minimized. The derivation of these integrals has been studied in several places [1, 3].

Our study is motivated by the discovery that the homogeneous TTM or Winslow grid generator produced folded grids in certain electrode configurations [2]. In these configurations the regions studied were roughly like the region between two concentric ellipses [see Figure 1a]. In the electrode problem the folded grid was 100 by 15. It was discovered

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COMMUNICATIONS IN APPLIED NUMERICAL METHODS, Vol. 7, 345–354 (1991)

HYBRID ADAPTIVE POISSON GRID GENERATION AND GRID SMOOTHNESS

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SUMMARY

A hybrid technique for adaptive grid generation using a variety of Poisson grid generators is described. The technique ensures that, when adaptivity functions are weak, the adapted grid reverts to an arbitrary specified base grid rather than to the grid produced by the homogeneous elliptic generator. The hybrid technique also serves to expose the weakness of the claim that elliptic grid generators produce smooth grids.

INTRODUCTION

Adaptive grid generation has been used frequently in recent years by investigators to obtain more accurate and efficient solutions to a variety of problems. This paper identifies one common shortcoming of adaptive elliptic methods, and presents a hybrid technique to overcome it. This simple technique also explains a common misconception regarding grid smoothness.

ADAPTIVE POISSON GRID GENERATION

Using the idea of equidistribution of some weight functions over the computational mesh, Anderson[1] showed that the Poisson grid generation scheme of Thompson, Thames and Mastin[2] (denoted as TTM herein) can be interpreted as a non-linear equidistribution scheme and extended TTM to include adaptivity. A variety of grid controls may be accommodated, with the grid control functions defined in terms of auxiliary functions introduced by Thomas and Middlecoff.[3] The method allows a relatively simple conversion of the ubiquitous TTM codes to solution adaptivity through the non-homogeneous terms.

However, this adaptive method (and others based on elliptic grid generators) has a serious shortcoming. Whenever the weighting function is weak, the generated grid reduces to that produced by the original Winslow[4] or homogeneous TTM[2] method. Thus, the grid will experience the same type of difficulties as that method. Thompson *et al.*[2] noted the tendency of the homogeneous method to pull grid lines away from any concave boundary. Even more seriously, Roache and Steinberg[5] demonstrated that, for a particular common class of geometry, the homogeneous method will produce folded grids. (See also the example calculations in the original Winslow[4] paper.)

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Variational Grid Generation[†]

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Recently, variational methods have been used to numerically generate grids on geometometric objects such as plane regions, volumes, and surfaces. This article presents a new method of determining variational problems that can be used to control such properties of the grid as the spacing of the points, area or volume of the cells, and the angles between the grid lines. The methods are applied to curves, surfaces, and volumes in three-dimensional space; then segments, plane curves, and plane regions appear as special cases of the general discussion. The methods used here are simpler and clearer and provide more direct control over the grid than methods that appear elsewhere. The methods are applicable to any simply connected region or any region that can be made simply connected by inserting artificial boundaries. The methods also generalize easily to solution-adaptive methods.

An important ingredient in our method is the notion of a reference grid. A reference grid is defined on a region that is simpler, but analogous to, the geometric object on which a grid is desired. Variational methods are then used to transfer the reference grid to the geometric object. This gives simple and precise control of the local properties of the grid.

I. INTRODUCTION

In this article we study the problem of using a computer program to automatically generate grids on curves, on surfaces, or in volumes in three-dimensional Euclidean space. Curves and surfaces in two-dimensional Euclidean space and segments will be included as special cases in the general discussion. The problem of grid generation has a long history and many important applications, which are described in [4]. We were motivated to study the grid generation problem because we were interested in using such grids in finite-difference codes that are used to solve partial differential equations. However, that applications area does not play a central role here.

Intuitively, a discrete grid on a curve is a sequence of points that divides the curve into pieces that are nearly straight line segments; a discrete grid on a surface is a set of points that divides the surface into approximate parallelograms (the grid need not be orthogonal); a discrete grid in a volume is a set of points that divides the volume into cells that are nearly parallelepipeds. In all cases,

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Mathematical Aspects of Numerical Grid Generation

Edited by José E. Castillo
San Diego State University

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PARAMETER ESTIMATION IN VARIATIONAL GRID GENERATION[1]

by

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Abstract

Two approaches to numerical variational grid generation use a linear combination of three variational problems to control the properties of the grid. Previously the parameters in the linear combination were determined by experimentation. Good estimates for these parameters can be obtained from simple model problems.

[1]This work was partially supported by ARO and AFOSR.

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GENERATING SUBROUTINE CODES WITH MACSYMA

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Abstract. The symbol manipulator MACSYMA is used as a high-level interface between the user and FORTRAN. MACSYMA is used to write numerical code for solving systems of ordinary differential equations.

Keywords. Symbol manipulation; automatic code generation.

INTRODUCTION

Languages such as FORTRAN provide valuable tools to the computer user, and such "mid-level" languages can be used to do sophisticated numerical computing. However, there are some problems which arise. One is that in FORTRAN all code is specific to the calculation at hand: array sizes must be set up in the code, and input to pre-written codes is severely limited. With FORTRAN code, it is basically "numbers in, numbers out". Equations cannot be changed without editing the code. This means that to write codes for solving many different systems of the same type, the user must make a "template file", copy it, and insert all array sizes and equations individually, which is highly inefficient. Another problem is that input and output for FORTRAN codes are not easily interpreted by those not familiar with the calculations in question. The user must often process output to make it understandable to others.

Both of these problems can be eliminated by the use of a high-level interface between users and FORTRAN code. The plan here is for the user to type in readily-understood expressions – statements and equations – which are used by a symbol manipulator (e.g. MACSYMA) to generate FORTRAN code; this in turn can be used to drive some standard FORTRAN code. Much of the intermediate information MACSYMA produces on its way to the FORTRAN code can be output to the user, who can then see results in the form of equations, rather than lists of numbers. Output from FORTRAN code can also be routed directly to graphics codes, to produce plots which give a much clearer picture of the results than lists of numbers could. The ultimate goal is to begin with "high-level" mathematics, physics, and engineering, and produce results that are easily understood by humans.

The purpose of this paper is to show, using a simple example, how MACSYMA can be used as an interface between the user and "canned" FORTRAN codes (in this case the code RKF45, a numerical ODE integrator).

PRELIMINARIES

Before looking at the MACSYMA code, it is helpful to know a little about a few MACSYMA commands, and how MACSYMA is programmed. This section gives a brief explanation of some of the commands used in the codes which follow.

One of the data types available in MACSYMA is the list. One way to make a list is to use the command *endcons*. This is done by producing an empty list, and then adding elements to the end of the list:

```
(c_1) list : [];
```

$$[] \qquad (d_1)$$

J. Symbolic Computation (1986) **2**, 213–216

Using MACSYMA to Write FORTRAN Subroutines†

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(*Received 2 January 1986*)

1. Introduction

This letter describes some ongoing work that uses the symbol manipulator MACSYMA to write FORTRAN subroutines which are incorporated into a large finite difference code that is used to solve boundary value problems for elliptic partial differential equations. The boundary value problems model the steady state of certain physical devices such as the electric field in a laser cavity or the flow around a blade in a turbine. The devices that interest us are those that occupy a fairly complicated region in three-dimensional space or, at best, have sufficient symmetry so that they can be modelled using a complicated two-dimensional region. The partial differential equations that are used to model the physics of the device are called the hosted equations. The hosted equations tend to be rather simple non-linear elliptic equations. However, our methods will apply to the most complicated hosted equations. The problem is complete when appropriate boundary conditions are specified. These problems are difficult to solve because of the complicated geometry of the region.

2. Overview of the Problem

Several important approaches to solving such problems are based on finding a change of coordinates that maps the given physical region into a rectangular region in logical space. Such a coordinate change then generates a grid in the physical region that corresponds to a rectangular grid in logical space. This approach now has a long history that is referenced in the papers listed below. Once such a transformation has been found, the hosted equation and the boundary conditions are transformed to the new coordinate system and then standard finite difference methods are applied to solve the problem. These numerical methods are described in our papers. What we will describe here is how a symbol manipulator is used to generate the FORTRAN subroutines that are used by the finite difference codes.

The regions that interest us are so complicated that it is often impractical or impossible to find an analytic change of coordinates that transforms the region to a rectangular region. Historically, practitioners in this area have used finite difference approximations

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In addition to the publications listed previously, which were directly supported by the subject contract, the continuation of this grid generation work initially funded by AFOSR has resulted in other significant publications. Besides the two books mentioned earlier, a sampling of related later work follows, especially those resulting from the AFWL contracts entitled "Adaptive Grids for RAVEN" (see Section G below).

Related Publications.

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Anomalies in Grid Generation on Curves*

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Attempts to use variational grid-generation methods to generate grids on certain surfaces of modest shape failed. There were sufficient points in the grids to well-resolve the surface, so the failures were not easily explained. Similar difficulties were found for variational grid generation on curves; those problems are caused by multiple solutions of the underlying non-linear algebraic equations. © 1990 Academic Press, Inc.

1. BACKGROUND

This paper describes several grid-generation anomalies discovered by the authors while using the variational techniques, described in Steinberg and Roache [9], to generate grids on surfaces. These surfaces are of modest shape (they are intended to model a stern wave behind a ship hull) and the grids being generated resolve the surfaces well. The anomalies manifest themselves as convergence problems. Grids are difficult or impossible to generate: for some coarse resolutions (to be expected); for many fine resolutions (not to be expected). For many intermediate resolutions, it is easy to generate excellent grids. Numerical experimentation fails to pinpoint the source of the difficulties. The surface grid-generation equations are a complicated system of two coupled quasi-linear partial differential equations that have a form similar to elliptic equations.

Some numerical experimentation shows that the analogous grid-generation code for curves has the same difficulties as the surface grid generator. This paper presents an analysis of the curve problem because it is simpler than the surface problem and

* This work was partially supported by the Office of Naval Research and the Air Force Weapons Laboratory. This is a modified version of AIAA Paper No. 88-3740, presented at the 1st National Fluid Dynamics Conference, Cincinnati, OH, July, 1988.

0021-9991/90 $3.00

Need for Control of Numerical Accuracy

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The need for the control of numerical accuracy in computational fluid dynamics (CFD) code solutions is reviewed in the light of current journal practice and experience with implementation of an editorial policy on the same subject published by the *Journal of Fluids Engineering*. Various actual objections to that policy are listed and responses are given. The general successes and particular difficulties experienced in the implementation of the policy are noted. The broader question of code verification, validation, and certification is considered. It is suggested that professional societies such as the AIAA and American Society of Mechanical Engineers may ultimately become involved in the task of certification of commercially available CFD codes.

I. Introduction

THIS paper, on the general philosophy and need for numerical accuracy control in computational fluid dynamics (CFD) codes, is based on experience with the implementation of an editorial policy statement by the American Society of Mechanical Engineers (ASME), published in the *Journal of Fluids Engineering (JFE)*.[1] The policy statement was conceived following the creation of the position of Associate Editor for Numerical Methods in the *JFE*, which formally recognized the special needs of this discipline. The ASME policy and supporting statements are reproduced in the Appendix. The rationale and needs for the policy statement are explained in the announcement. The *JFE* had previously published and had many years of experience with a similar requirement for uncertainty analysis in experimental papers. Following our early experience with this new policy, a similar policy was also adopted by the ASME's *Journal of Heat Transfer*. The general subject of control of numerical accuracy has become something of a "hot topic," with special reference to the National Aero-Space Plane, a session at the AIAA 1989 Thermophysics Conference, ASME sessions at the 1988 and 1989 Winter Annual Meetings, and by the Texas Institute for Computational Mechanics workshop on the slightly broader topic of reliability in computational mechanics in October 1989.

II. Resistance and Objections

Although Roache et al.[1] thought that the policy statement and the editorial requirement were quite mild, it was not universally welcomed. Objections were offered by some of the other editorial board members and by other members of the professional community from whom I solicited comments in the months following the publication of the statement. Some of these objections, all of which are actual (i.e., not straw-man objections), are listed below, together with my responses.

Objection 1

It is too expensive of computer time to do mesh doubling calculations in order to ascertain grid convergence.

There are, of course, other ways to ascertain grid convergence than the straightforward method of grid doubling. In fact, this is probably the most reliable method available, but there are other approaches, as briefly touched upon in the original policy statement. If the cost of computer resources is not a problem to the researcher, this is certainly the easiest approach to take. However, if computer resources are a problem, there are other methods that are not intensive users of computer time. It seems that the greater objection for doing grid convergence studies is the fact that it requires a bit of conscientious work on the part of researchers.

Also, if it is argued that it is simply too expensive to do any kind of control of numerical accuracy, then I would argue that the author simply cannot be in this CFD business. After all, if you do not have a wind tunnel you cannot do experimental testing. My impression of the situation is actually worse than this. Journal articles in the late 1960s and early 1970s commonly predicted high resolution accuracy runs when the next generation of computers became available. But for the most part they have not been used that way. Generally the tremendous advance of computing power has been used to produce more mediocre papers rather than fewer reliable ones.

Objection 2

Some exception to the policy should be made for expensive calculations, particularly three-dimensional turbulent studies.

I do not think that the overall cost of the computations should be a consideration. It seems clear that the incremental cost of performing a grid convergence test should be normalized by the cost of the base case. In this sense it is cheaper to validate the grid convergence on a three-dimensional problem than on a two-dimensional problem, presuming that the incremental work involves an extra coarse grid computation. This again relates to the first point, which states that it is not necessary to do a grid doubling in order to ascertain some index of numerical accuracy. A grid halving is also appropriate. Of course, the advantage lies in doing a grid doubling test because the error bounds will be sharper.

Objection 3

Turbulence modeling, rather than the numerical solution of the partial differential equations, is the real determinator of accuracy.

My response is, yes and no. Accuracy is a question to be addressed even for laminar flow calculations, wherein the constitutive equations are not in doubt. The discretization error does not disappear just because one uses a turbulence model! Our point in the *JFE* policy statement, and the first criticism which our evaluation committee made at the 1980/81 Stanford meeting on complex turbulence flows,[2] is that one cannot evaluate different turbulence models unless one first satisfies grid convergence. There are yet more considerations

Presented as Paper 89-1669 at the 24th AIAA Thermophysics Conference, Buffalo, NY, June 12-14, 1989; received July 8, 1989.

*President. Senior Member AIAA.

AIAA 90-0581

THE INFLUENCE OF SWEEP ON DYNAMIC STALL PRODUCED BY A RAPIDLY PITCHING WING

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28th Aerospace Sciences Meeting

January 8-11, 1990/Reno, Nevada

THE INFLUENCE OF SWEEP ON DYNAMIC STALL PRODUCED BY A RAPIDLY PITCHING WING

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Abstract

The influence of sweep on deep dynamic stall of a rapidly pitching swept wing at low Mach number with laminar flow has been investigated through the use of numerical flow simulations. The problem involves the modeling of a wind tunnel test section in which the wing spans the tunnel. The flow Reynolds number is 10,000, free stream Mach number is 0.2, the reduced frequency is equal to 0.3, and the sweep angle is 30 degrees. The solution of the full unsteady three-dimensional compressible Navier Stokes equations was obtained on the CRAY-2 supercomputer through use of an implicit finite difference Approximate Factorization algorithm coupled with a non-orthogonal moving grid. The sweep effects have been determined by comparing the unswept (2-D) and swept (3-D) solutions. Sweep tends to delay the onset of dynamic stall and reduce the magnitude of unsteady aerodynamic loads. However, the intensity of these effects vary significantly along the span of the wing. Sweep was also found to inhibit the growth of the secondary stall vortex and its contribution to aerodynamic forces. The side tunnel walls tend to alter the behavior of the stall vortex or prevent its formation.

I. Introduction

History

Around 1968 design engineers in the helicopter industry observed that the lift generated by a helicopter blade in experiments was much higher than the lift predicted using conventional aerodynamics. Harris and Pruyn [1] realized the importance of unsteady aerodynamics in resolving this discrepancy. Concurrently, Ham and Carelick [2] observed that the extra lift was associated with a vortex which formed by rapid pitching of an airfoil during the unsteady motion. Ham [3]

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COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING 78 (1990) 313–329
NORTH-HOLLAND

ON THE INVERTIBILITY OF THE ISOPARAMETRIC MAP

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Received 12 February 1989

Most 3D finite difference or finite element codes make use of hexahedral cells having six faces, eight corners and twelve edges. Interpolation between grids makes use of the isoparametric map from a uniform logical space to a given hexahedral cell. In two dimensions, it is well-known that the isoparametric map is invertible if and only if the Jacobians at the four cell corners are positive. The corresponding conjecture in three dimensions is shown to be false and alternative tests for positivity of the Jacobian are investigated.

1. Properties of the Jacobian in $\mathbb{R}^2$

Following Strang and Fix [1], the isoparametric mapping from the unit square $U_2 = \{(\xi, \eta) \mid 0 \leq \xi, \eta \leq 1\}$ to a quadrilateral Q in $\mathbb{R}^2$ (Fig. 1) is given by the pair of bilinear forms

$$x(\xi, \eta) = x_1 + (x_2 - x_1)\xi + (x_3 - x_1)\eta + (x_4 - x_3 - x_2 + x_1)\xi\eta \,, \tag{1}$$

$$y(\xi, \eta) = y_1 + (y_2 - y_1)\xi + (y_3 - y_1)\eta + (y_4 - y_3 - y_2 + y_1)\xi\eta \,. \tag{2}$$

The isoparametric map is a special case of the well-known 'shearing transformation' used in algebraic grid generation in which all four sides of the given region are straight lines. The grid

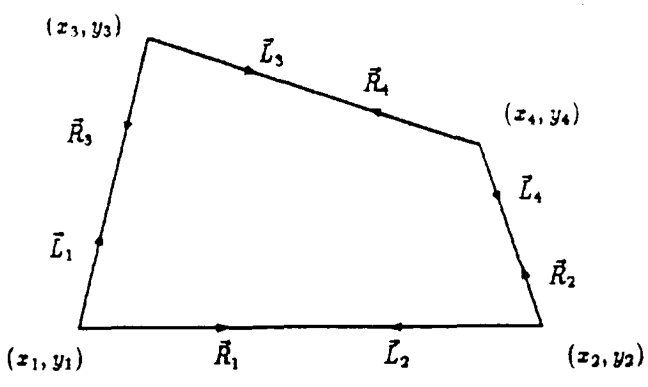

Fig. 1. 2D isoparametric map to a quadrilateral.

* This work was partially supported by funding from Sandia National Laboratories, Albuquerque NM, U.S.A.

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COMPLETED RICHARDSON EXTRAPOLATION

by

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Abstract

Abstract: The Richardson extrapolation method, which produces a 4th order accurate solution on a subgrid by combining 2nd order solutions on the fine grid and the subgrid, is "completed", in the sense that a higher order accurate solution is produced on all the fine grid points.

INTRODUCTION

In his classic paper in 1910, Richardson [1] presented a method for obtaining 4th order accurate solutions. The method, known variously as Richardson extrapolation, extrapolation to the limit, deferred approach to the limit, or iterated extrapolation [2] takes separate 2nd order solutions on a fine grid and on the subgrid formed of alternate points, and combines them to obtain a 4th order solution on the subgrid. It is also the basis of Romberg integration [3].

The usual assumptions of smoothness apply, as well as the assumption (or perhaps presumption) common to finite difference methods that the local error is indicative of global error. The method must be used with considerable caution, since it involves additional assumptions of monotone truncation error convergence in the mesh spacing h (which may not be valid for coarse grids) and since it magnifies machine round-off errors and incomplete iteration errors [2,4]. In spite of these caveats, the method is extremely convenient to use compared to forming and solving direct 4th order discretizations, which involve more complicated stencils, wider band-width matrices, special considerations for near-boundary points and non-Dirichlet boundary conditions, additional stability analyses, etc., especially in nonorthogonal coordinates which generate cross-derivative terms and generally complicated equations. Such an application was given in [5] by the first author. The method is in fact oblivious to the

*President and Chief Scientist.
**Staff Scientist II.

E. PROFESSIONAL PERSONNEL ASSOCIATED WITH THE RESEARCH EFFORT

Dr. Patrick J. Roache, Principal Investigator
Dr. Stanly Steinberg
Dr. Jose' Castillo
Mr. Paul Sery

F. INTERACTIONS (COUPLING ACTIVITIES)

(1) PRESENTATIONS AT MEETINGS, CONFERENCES, SEMINARS

PRESENTATIONS

"Computers vs. Algorithms", Symposium on the Impact of Large-Scale Computing on Air Force Research and Development, 4-6 April 1984, Air Force Weapons Laboratory, Albuquerque, NM.

"Interactive Electric Field Calculations for Lasers", AIAA 17th Fluid Dynamics, Plasma Physics, and Lasers Conference, 25-27 June 1984, Snowmass, CO.

"Computers vs. Algorithms", Engineering Faculty Seminar, 5 November 1984, University of Canterbury, Christchurch, New Zealand.

"Symbolic Manipulation and Computational Fluid Dynamics", Engineering Faculty Seminar, 7 November 1984, University of Canterbury, Christchurch, New Zealand.

"Application of a Single-Equation MG-FAS Solver to Elliptic Grid Generation Equations (Sub-grid and Super-grid Coefficient Generation)", Second Copper Mountain Conference on Multigrid Methods, 1-3 April 1985, Copper Mountain, CO.

"Symbolic Manipulation and Computational Fluid Dynamics", Engineering Faculty Seminar, 2 May 1985, Univ. California at Davis.

"Symbolic Manipulation and Computational Fluid Dynamics", Applied Mathematics Seminar, 7 May 1985, Sandia Labs., Livermore, CA.

"A New Approach to Grid Generation Using a Variational Formulation", AIAA 7th Computational Fluid Dynamics Conference, 15-17 July 1985, Cincinnati, OH.

"The ELF Codes: Electrode Design for Lasers and Switches", Invited Paper, CTAC-85 Conference, 25-28 August 1985, Melbourne, Australia.

"PDE Discretization on Subgrids and Supergrids", SIGNUM Meeting, 8 December 1985, Albuquerque, NM.

"A Tool Kit of Symbolic Manipulation Programs for Variational Grid Generation", AIAA Aerospace Sciences Meeting, 6-9 January 1986, Reno, NV.

"Symbolic Manipulation and Computational Fluid Dynamics", Invited Presentation, NSF Workshop on Computational Engineering, 24-25 June 1986, NSF San Diego Supercomputer Center, San Diego, CA.

"The ELF Codes", Spectra Technologies, Seattle, WA, 17 July 1986.

"Grid Generation in Finite Analysis", Applied Mechanics Research Seminar, Mechanical Engineering Department, University of New Mexico, February 17, 1987, Albuquerque, NM.

"Symbolic Generation of Strong Conservation Forms for General Coordinate Finite Difference Codes", Invited Presentation, Symposium on Symbolic Computation in Heat Transfer and Fluid Mechanics, ASME Winter Annual Meeting, Chicago, Ill. Dec. 1988.

(1) CONSULTATIVE AND ADVISORY FUNCTIONS

P. J. Roache and S. Steinberg consulted with Dr. R. L. Rapagnani and other personnel at AFWL on various problems involving grid generation during 1984-1986.

G. NEW DISCOVERIES, INVENTIONS, PATENTS, SPECIFIC APPLICATIONS

No inventions or patents have resulted from this work.

The 2-D and 3-D adaptive grid generation algorithms developed in this work and the preceding AFOSR contract have been applied in the ELF codes (ELectric Field) developed at Ecodynamics under subcontract to Tetra Corporation for the Air Force Weapons Laboratory (now Phillips Laboratory, Kirtland AFB, NM). These codes are under fairly extensive use at Phillips, at Tetra Corporation, and at university and for-profit DoD contractors for the design and optimization of laser electrodes and high power switches. Applications are in the Pulsed Power area, including SDI research and development. Over 25 copies of ELF have been sold commercially, many to government and Air Force contractors, as well as the Canadian Atomic Energy Commission. The ELF codes were also the utilized in an SBIR Phase I contract from AFOSR to Ecodynamics on "Design Optimization of Systems Governed by Partial Differential Equations".

The 2-D and 3-D adaptive and variational grid generation algorithms developed in this work were also the basis for SBIR Phase I and II contracts to Ecodynamics from the Air Force Weapons Laboratory (now Phillips Laboratory, Kirtland AFB, NM) entitled "Adaptive Grids for RAVEN". The IMPLICIT RAVEN code developed under this contract, as well as the earlier RAVEN code, are accessible on the Cray-2 system library at Phillips and are available for use by government contractors for the analysis of problems in subsonic and supersonic aerodynamics and well as chemical lasers. The IMPLICIT RAVEN code has also been marketed commercially.

These grid generation algorithms were also the basis for SBIR Phase I and II contracts to Ecodynamics from the U.S. Army (AMSAV) on "Dynamic Stall Control", specifically focused on retreating helicopter blade dynamic stall. (Phase II has just recently started.)

They were also the basis for a contract from the U.S. Navy (ONR) on "Computational Ship Waves" with specific focus on free surface calculations behind a transom stern. Dr. R. Yeung of University of California at Berkeley and his graduate students have highly tuned our variational surface grid generation method (utilizing a reference grid to control target grid properties) for free surface flows with great success, and have published their results recently in

International Journal for Numerical methods in Fluids.

These grid generation algorithms were also the basis for Phase I SBIR contracts from the U.S. Navy (NUSC) on "Unsteady Flow in a Torpedo Shuttleway", from the U.S. Navy (NAVSEA) on "Computational Modeling of 3-D Unsteady Flow", specifically focused on simulation of flow in gas turbine diffusers, and from the National Science Foundation (Mathematics Division) on "Robust and Fast Numerical Grid Generation". The Phase II award decisions for the last two have not yet been made.

Ecodynamics is presently planning to market these grid generation modules interfaced to the two most used packages in the aerodynamics community, GRIDGEN and EAGLE.